

Superconducting d -wave junctions: The disappearance of the odd ac components

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We study voltage-biased superconducting planar d -wave junctions for arbitrary transmission and arbitrary orientation of the order parameters of the superconductors. For a certain orientation of the superconductors the odd ac components disappear, resulting in a doubling of the Josephson frequency. We study the sensitivity of this disappearance to orientation and compare with experiments on grain boundary junctions. We also discuss the possibility of a current flow parallel to the junction.

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Some of the hole-doped high- T_c cuprates show features that cannot be explained using an s -wave order parameter.^{1,2} Instead various phase-sensitive experiments involving Josephson junctions suggest that the order parameter changes sign at certain regions of the Fermi surface. The outcome of these and other experiments makes d -wave symmetry a particularly interesting candidate for the symmetry of the superconducting order parameter in the high- T_c cuprates.¹

Hu's prediction of midgap states (MGS) at interfaces/surfaces of d -wave superconductors³ called for a reinvestigation of a number of transport problems involving d -wave superconductors. This reinvestigation has to some extent been carried out, starting with the normal metal-superconductor (NS) junction,^{4,5} followed by the dc Josephson effect⁶⁻⁸ and the ac Josephson effect.^{9,10} It has been found that the zero-energy MGS influence the current-voltage relation (the NS-case and the ac Josephson effect), the temperature dependence, and the current-phase relation (the dc Josephson effect).

The origin of MGS is due to normal scattering of the quasiparticles at interfaces/surfaces. Since the quasiparticle changes its momentum when scattered, it will in the d -wave case experience a different order parameter after scattering. When there is a sign change of the order parameter after scattering, a bound state is formed at the interface/surface of the superconductor.³

In this paper we investigate the ac Josephson effect in planar d -wave junctions, calculating the first Fourier components of the current. The order parameter $\Delta(\theta)$ for an anisotropic superconductor depends on the angle θ of incidence for the quasiparticle approaching the junction. For the d -wave case the order parameter is taken to be $\Delta(\theta) = \Delta_0 \cos[2(\theta - \alpha)]$, where α is the angle of orienta-

tion of the superconducting order parameter with respect to the junction interface as explained in Fig. 1. The cases $\alpha = 0$ and $\alpha = \pi/4$ correspond to $d_{x^2-y^2}$ and d_{xy} symmetry, respectively. For the s -wave case, $\Delta(\theta) = \Delta_s$.

For conventional superconducting junctions with s -wave electrodes the frequency of the non-stationary Josephson current is $\omega_J = 2eV/\hbar$. This means that the Josephson current perpendicular to the junction can be decomposed into components with frequency parts $m\omega_J$ (m is an integer):^{11,12}

$$I(t) = \sum_m I_m e^{im\omega_J t}. \quad (1)$$

The zero-frequency component has been studied recently for the d -wave case.¹⁰ In this paper we extend the analysis to include the nonzero frequency parts of the current.

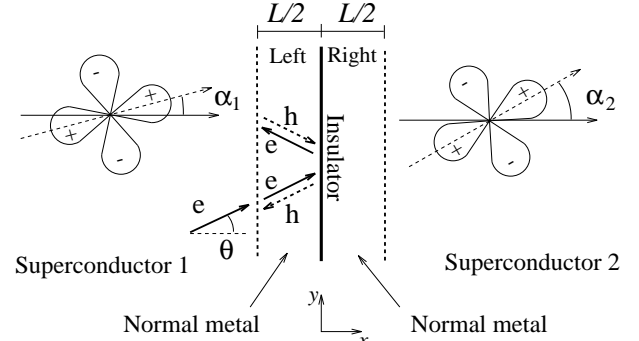


FIG. 1. Layout of the junction. The superconductors can be rotated to an angle $\alpha_{1,2}$. The strength of the barrier can be tuned all the way from the ballistic to the insulating case.

In the s -wave case one finds that all components I_m in Eq. (1) are nonzero although they decrease with increasing m . This is not necessarily the case when d -wave superconductors are introduced in the junction. Consider the d -wave junction and let the order parameter of the left (right) superconductor be $\Delta_1(\theta)$ [$\Delta_2(\theta)$]. For orientations of the superconductors where $\Delta_1(\theta) = \Delta_1(-\theta)$ (the case for s -wave and $d_{x^2-y^2}$ orientation of the left superconductor) and $\Delta_2(\theta) = -\Delta_2(-\theta)$ (d_{xy} orientation of the right superconductor) we find that $I_m = 0$ for odd m and therefore the Josephson frequency is doubled. This doubling of the Josephson frequency has previously been inferred from the stationary Josephson effect,¹³ where one can show that in the situation described above the Josephson current is π -periodic in the phase rather than

2π -periodic. This change of period in the phase would then change the Josephson frequency accordingly.

Considering the nonstationary Josephson effect, we may calculate the Fourier components and explore the sensitivity of the odd ac components to deviation from orientations where disappearance of the odd ac components occur. This is the main subject of this paper and is not possible to treat within the framework of the stationary Josephson effect.

In passing, we note that the disappearance of the odd ac components is not related to the presence of MGS itself; even for the ballistic junction (when there are no MGS present) the odd ac components disappear in the situation described above.

In our calculation self-consistency of the superconducting order parameter is not fulfilled. Recent investigations in the tunneling limit have considered self-consistency and found that interface states with nonzero energy appear along with the zero-energy MGS.⁹ In this paper we neglect these effects.

The system that we consider is shown in Fig. 1. Two superconductors are separated by a barrier represented by a scattering matrix, which for electrons is

$$S_e(\theta) = \begin{pmatrix} r(\theta) & t(\theta) \\ t(\theta) & -r^*(\theta)t(\theta)/t^*(\theta) \end{pmatrix}. \quad (2)$$

The scattering matrix for holes is $S_h(\theta) = S_e^*(\theta)$. The normal reflection at the barrier changes the angle from θ to $\bar{\theta} = \pi - \theta$. All barred quantities in this paper are related to $\bar{\theta}$.

We solve the time-dependent Bogoliubov-de Gennes equation for d -wave superconductors piecewise in each region. The details of the method can be found in e. g. Ref. 10. The order parameter is assumed to be

$$\Delta(\mathbf{k}, \mathbf{x}, t) = \begin{cases} \Delta_1(\theta), & x < -L/2 \\ 0, & |x| < L/2 \\ \Delta_2(\theta)e^{i(\phi_0 + 2eVt/\hbar)}, & x > L/2. \end{cases} \quad (3)$$

The overall phase is not important and we therefore choose Δ_1 real and let the phase difference between the superconductors be ϕ_0 . In Eq. (3) it is understood that we only consider \mathbf{k} -vectors with $|\mathbf{k}| = k_F$.

Solving the scattering problem, we inject an electron-like quasiparticle from the left superconductor at energy E and angle θ . Since there is a voltage bias over the junction, the quasiparticle goes through multiple Andreev reflections (MAR). The barrier is modeled as a δ -function potential of strength H with transmission amplitude $t(\theta) = i \cos \theta / (i \cos \theta - Z)$ and reflection amplitude $r(\theta) = Z / (i \cos \theta - Z)$, where Z is defined as $Z = 2mH/\hbar^2$. Our calculations include normal regions to the left and to the right of the barrier, but the length L is put to zero at the end of the calculation. Therefore, our method follows closely the one presented by Averin and Bardas.¹² However, the same results would have been obtained if we had used the method of Bratus, Shumeiko, and Wendin.^{11,14}

It is convenient to calculate the current in the normal region to the left of the barrier. The wave function in this region is

$$\Psi \rightarrow \sum_n \begin{pmatrix} a_{2n} e^{i\mathbf{k} \cdot \mathbf{x}} + d_{2n} e^{i\bar{\mathbf{k}} \cdot \mathbf{x}} \\ b_{2n} e^{i\mathbf{k} \cdot \mathbf{x}} + c_{2n} e^{i\bar{\mathbf{k}} \cdot \mathbf{x}} \end{pmatrix} e^{-i(\frac{E_{2n}t}{\hbar} + n\phi_0)}, \quad (4)$$

where the momentum is defined by $\mathbf{k} = (k_x, k_y) = k(\cos \theta, \sin \theta)$ and $\bar{\mathbf{k}} = (-k_x, k_y) = k(\cos \bar{\theta}, \sin \bar{\theta})$. We have introduced the energy $E_n = E + neV$, where n is an integer. Note that we have separated out the phase difference ϕ_0 between the superconductors, making the coefficients a , b , c , and d independent of ϕ_0 . Matching the wave functions of the different regions one gets the coefficients a , b , c , and d as written down in Ref. 10.

The next step is to calculate the current by inserting the wave function into the following formula for the current density

$$j = \frac{e\hbar}{m} \sum_n \tanh\left(\frac{-E_n}{2k_B T}\right) \text{Im}\{u_n^* \nabla u_n + v_n^* \nabla v_n\}, \quad (5)$$

where (u_n, v_n) is the solution of the BdG equation. The sum is over all incoming electron-like quasiparticles for both negative and positive energies. There are different ways of writing the current density. Using the completeness relation for solutions of the BdG equation¹⁵ one can show that Eq. (5) is equivalent to the current formulas written down in previous work.^{11,16,17}

Including also the left-moving quasiparticles we can determine the expression for the ac components I_m in Eq. (1):

$$\begin{aligned} \frac{I_m(V)}{\sigma_0} &= C_m(V) e^{i(m\phi_0 - \alpha_m)}, \quad m \neq 0 \\ C_m(V) &= \sqrt{A_m^2(V) + B_m^2(V)}, \quad \alpha_m = \arctan \frac{B_m(V)}{A_m(V)}, \\ \sigma_0 &= L_y \frac{2^{5/2} e m^{1/2} E_F^{1/2} \Delta_0 D}{\hbar^2}, \end{aligned} \quad (6)$$

where $D = \int d\theta |t|^2 \cos \theta / 2$ is the transmission probability through the barrier averaged over all angles θ , and L_y is the junction length in the y -direction.¹⁸ In Eq. (6) we introduced $A_m(V)$ and $B_m(V)$ which are the coefficients in the cosine and sine expansion of the ac current. The coefficients are defined as

$$\begin{aligned} A_m(V) &= \frac{1}{4D} \int_{-\pi/2}^{\pi/2} d\theta \cos \theta \int_{-\infty}^{\infty} \frac{dE}{\Delta_0} \tanh\left(\frac{-E}{2k_B T}\right) \\ &\quad \times \sum_{\tau} \tau N_{\tau}(E) \text{Re}\{T^{\tau}(E, \theta, m)\}, \\ B_m(V) &= -\frac{1}{4D} \int_{-\pi/2}^{\pi/2} d\theta \cos \theta \int_{-\infty}^{\infty} \frac{dE}{\Delta_0} \tanh\left(\frac{-E}{2k_B T}\right) \\ &\quad \times \sum_{\tau} N_{\tau}(E) \text{Im}\{T^{\tau}(E, \theta, m)\}, \end{aligned} \quad (7)$$

where $\tau = + (-)$ means right (left) movers, $N_\tau(E, \theta)$ is the bulk superconducting density of states evaluated in superconductor 1 (2) for $\tau = + (-)$, and

$$T^\tau(E, \theta, m) = \sum_{n=-\infty}^{\infty} (a_{2n+2m,\tau}^* a_{2n,\tau} - d_{2n+2m,\tau}^* d_{2n,\tau} + b_{2n+2m,\tau}^* b_{2n,\tau} - c_{2n+2m,\tau}^* c_{2n,\tau}). \quad (8)$$

The phase $m\phi_0 - \alpha_m$ in Eq. (6) defines the (m -dependent) time when the measurement is started, and may not be easily observed in a transport experiment. To illustrate our point that I_m (where m is an odd number) disappears for certain orientations it is enough to plot the amplitude $C_m(V)$.

We now investigate the ac components. For s -wave superconductors we have the ac Josephson effect where the Josephson frequency is ω_J . In the case of d -wave superconductors this may not be true, as discussed above. For the case $d_{x^2-y^2}/d_{xy}$ we find $C_1 = 0$ and $C_2 \neq 0$, meaning that the Josephson frequency for this configuration is $2\omega_J$. Decreasing α_2 from $\pi/4$ (the case d_{xy}), the magnitude C_m of the odd ac components increases from zero (and therefore reestablishes the ordinary Josephson frequency ω_J) until α_2 reaches 0, in which case the situation more resembles the s -wave case. To understand this effect we study the case $d_{x^2-y^2}/d_{xy}$. The expression for the current involves an integration over both positive and negative injection angles θ . We may explicitly calculate the current for positive and negative angles separately, and then add them to get the final result. When changing the angle θ to $-\theta$ we must change the phase ϕ_0 between the superconductors by π , because $\Delta_2(-\theta) = -\Delta_2(\theta) = \Delta_2(\theta)e^{i\pi}$ (meaning $\phi_0 \rightarrow \phi_0 + \pi$). The effect of this is seen in the wave function in Eq. (4), where we get an extra phase $-in\pi$. This phase, separated out together with ϕ_0 , will pass through the calculation and finally show up in the expression for the current:

$$I(V, t) = \sum_m (I_m(V, \theta > 0) + I_m(V, \theta < 0)) e^{im\omega_J t} \\ = \sum_m I_m(V, \theta > 0) (1 + e^{im\pi}) e^{im\omega_J t}, \quad (9)$$

where the amplitudes $I_m(V, \theta > 0)$ [$I_m(V, \theta < 0)$] now are defined with an integration over positive (negative) angles only. The factor $(1 + e^{im\pi})$ is zero for odd m and two for even m . This implies a doubling of the Josephson frequency for the case $d_{x^2-y^2}/d_{xy}$.

We present the ac components for different configurations of the superconductors and three different barrier strengths Z . The plots are shown in Fig. 2, and are only for $V > 0$ since one can show that $I(-V) = -I(V)$. For the $d_{x^2-y^2}/d_{xy}$ junction we only plot the first non-zero amplitude C_2 . For the $d_{x^2-y^2}/d_{\alpha_2 \neq \pi/4}$ junction we plot the components C_1 and C_2 since they are both non-zero.

The results show that the amplitude C_1 decreases smoothly as the angle α_2 is increased from 0 to $\pi/4$.

There is subharmonic gap structure (SGS) for the case of non-zero barrier strength at the same voltages as in the s -wave case [see Figs. 2(b) and 2(c)].¹⁶ Angular averaging partly washes out the SGS.¹⁰ There is no SGS for the ballistic case $Z = 0$ at zero temperature [see Fig. 2(a)].¹⁶

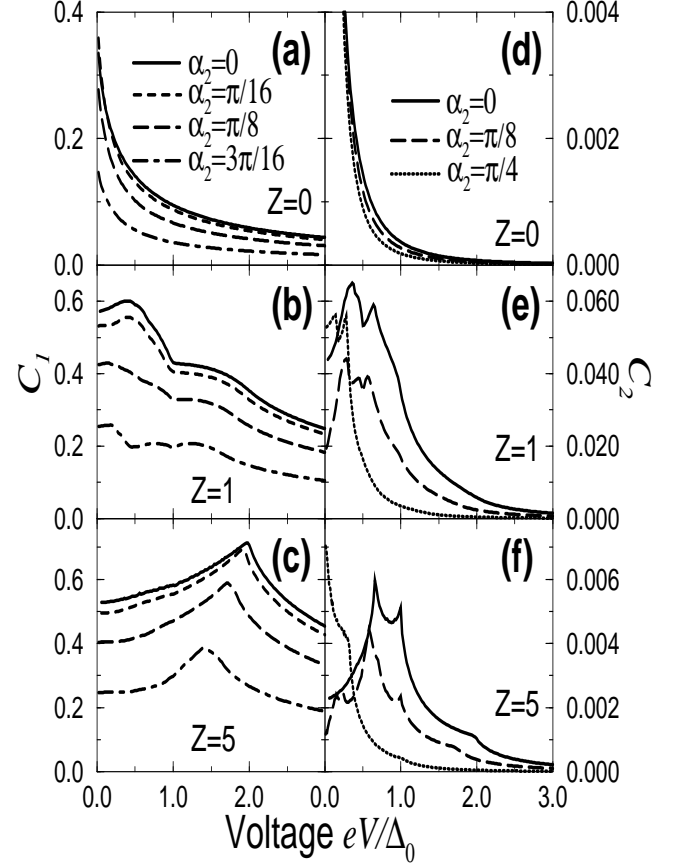


FIG. 2. Here we show the first two Fourier components as a function of voltage for three different barrier strengths Z . The orientation of the left superconductor is fixed at $\alpha_1 = 0$, while we vary the orientation of the right superconductor from $\alpha_2 = 0$ to $\alpha_2 = \pi/4$. The first component C_1 is identically zero for $\alpha_2 = \pi/4$ as explained in the text. Zero temperature is assumed.

Considering the second Fourier component C_2 , we first note that this component is much smaller than C_1 simply because C_2 corresponds to a higher order term in the expansion of the current in Eq. (1). The curves depicted in Figs. 2(e) and 2(f) again show SGS [no SGS in the ballistic case $Z = 0$ shown in Fig. 2(d)].¹⁶ When α_2 is close to $\pi/4$ and Z is large [see Fig. 2(f)], MGS clearly influence the curves of C_2 , resulting in an increase in C_2 for small voltage. MGS appear as resonances in the scattering states of Eq. (4) when the order parameter experienced by the quasiparticle changes sign after normal reflection at the barrier. Because of the large density of states at the gap, a quasiparticle trajectory passing through the MGS as the one depicted in Fig. 3 will give rise to a large contribution to the current. The resonant trajectory originates from the gap edge only when $3eV = \Delta_1 = \Delta_0 \cos 2\theta$ as seen in Fig. 3, meaning that

the upper limit for this particular process is $\Delta_0/3$.

Another quasiparticle trajectory passing through MGS is the one travelling back and forth within the gaps twice instead of six times as shown in Fig. 3. This process will give rise to a smaller current contribution to C_2 than the one shown in Fig. 3 for the following reason. Calculating C_2 we study energies E_{2n} and E_{2n+4} . For the process corresponding to $eV = \Delta_0 \cos 2\theta$, E_{2n+4} will be above the gap region, and therefore this process will be subject to two additional non-perfect (out of gap) Andreev reflections which suppress the contribution.

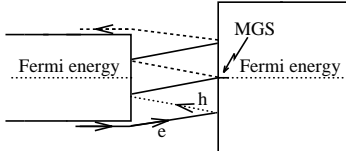


FIG. 3. The trajectory above gives rise to a large amplitude of the second component C_2 at small voltages, see Fig. 2(f). There is a resonance when the trajectory starts from the gap edge of the left superconductor, hits MGS, and finally ends at the gap again.

The condition $eV = \Delta_1 = \Delta_0 \cos 2\theta$ for the process shown in Fig. 3 does not depend on Δ_2 . This means that SGS corresponding to this process is present for all angles α_2 but the amplitude is smaller when $\alpha_2 \neq \pi/4$ since the resonant MGS do not occur at as many injection angles θ in this case. For $\alpha_2 = 0$ the structure is absent since there is no MGS in this case. Larger transmission (smaller Z) broadens MGS, making the effects of MGS less drastic, as seen when comparing Fig. 2(e) with Fig. 2(f). The first component C_1 shows no increase in amplitude at small voltages. Actually, there is similar SGS but this is smaller in amplitude than the ordinary background and does not dominate in the same way as for C_2 .

Considering the case of two d_{xy} superconductors, we get a phase shift of π in both superconductors when we let $\theta \rightarrow -\theta$, leading to no overall phase difference. Therefore the first ac component C_1 does not vanish in this case.

In experiments on high- T_c $d_{x^2-y^2}/d_{xy}$ grain boundary junctions,¹⁹ Shapiro steps have been found at voltages corresponding to a Josephson frequency of $2\omega_J$. As pointed out in Ref. 19 this effect may be explained by assuming that parallel junctions are formed at the grain boundary. According to our results it is possible that the doubled Josephson frequency is due to d -wave symmetry of the order parameter.

Very recently, it has been shown that there is a nonzero ground state current parallel to the junction²⁰ in the stationary case (zero voltage) for a s/d_{xy} junction. Inspired by these investigations, we have used our formalism to calculate the parallel current for the non-stationary case. For junctions with two d -wave superconductors we find both time-independent ($m = 0$) and time-dependent ($m \neq 0$) currents in the general case. For the y -direction current the even components disappear in the $d_{x^2-y^2}/d_{xy}$ geometry while the odd components are non-zero. This

happens because we get a minus sign between the two terms in Eq. (9) instead of the plus sign, making the x -direction and the y -direction currents complementary. This resembles the stationary case where the parallel current appears when the perpendicular current is zero.²⁰

Also for the N/d_α junction we find a time independent ($m = 0$; no ac in the NS case) current density in the y -direction at $x = 0$ if the up/down symmetry of the junction is broken by the order parameter, which is the case when the angle α has a value between 0 and $\pi/4$. For $\alpha = 0$ and $\alpha = \pi/4$ the current density in the y -direction is zero. The N/d_α case has recently been discussed.²¹ One notes that even for an asymmetric s -wave order parameter there are current contributions in the y -direction for the NS case.

In summary, we have calculated the ac components for voltage biased d -wave junctions. We find that the odd ac components of the current in the x -direction vanish if the orientations of the d -wave superconductors is $\alpha_1 = 0$ and $\alpha_2 = \pi/4$. For this case the Josephson frequency is doubled, which has also been found in experiments on grain boundary junctions.¹⁹ The reason for this effect is that the contributions from injection angles $+\theta$ and $-\theta$ have exactly the same magnitudes, but opposite signs. The angle average will then cancel the odd components. We have also discussed the possibility of current flow in the direction parallel to the junction.

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